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This is a progress report for the contract:: Novel Methods for Simulation of Large electromagnetic Structures. The work conducted under this contract is to develop new methods for speeding up electromagnetic simulation codes. Specifically, wavelet, multipole methods, and non-unifrom grid fast Fourier transform methods, are used.

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Novel Methods for Simulation of Large Electromagnetic Structures: Final Report

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Abstract

The purpose of this contract was to apply various mathematical techniques for speeding up electromagnetic simulation codes to present day commercial codes. The techniques to be investigated in the original contract were: wavelet methods, the non-uniform fast Fourier transform, and multipole methods. As the contract evolved, changes were made in two ways: first, the specific techniques investigated changed; second, the contract was modified to incorporate portions of another MAFET contract, which was part of the larger industrial consortium. That contract was terminated after its second year of funding due to budget constraints. As a result, this contract supported the remainder of that contracts work. Details are given as to the specific work performed, goals achieved, and future work to be carried out.

1 Summary of Work Performed

The work carried out under this contract is broken out into three main sections: wavelet methods, improvement of matrix condition numbers, and fast package models. Eachof these is described in more detail in later sections. Brief summaries of the activities are now given.

1.1 Wavelet Methods

The first half of the contract (18 months) concentrated on using wavelet methods to speed up the matrix solve of moment method matrices. Moment methods are the principal technique used for solving electromagnetic planar circuit problems. (The other major technique of choice, finite elements, is more popular with packaging problems. It is examined in the packaging simulation section of this contract.) The investigation concentrated on getting the wavelet methods to work on commercial codes. We concentrated on HP-EEsof's Momentum product. They gave us a copy of the code in which we could get at the matrices being generated in the solve portion of the numerical engine. We then examined converting the matrices to a wavelet basis, and solving the resulting matrix in the wavelet basis. We had hoped that the solve would be extremely fast, owing to the matrix being made more sparse. Unfortunately, the condition number of the matrices were poor. A poorly conditioned matrix cannot be solved by iterative techniques quickly, as the solve time goes as the condition number. Indeed, in extreme cases, the solver will never converge, when the finite precision arithmetic of a computer is included.

We therefore had to develop a way of working with the poorly conditioned matrices. Fortunately, the structure of the matrices after they have been converted to a wavelet basis permits a fast solve, even though they are badly conditioned. A standard solution technique for matrices is the LU decomposition method. Indeed, this is the standard method used in commercial moment method codes. If the matrix has N entries, the solve time goes as $\vartheta(N^3)$. However, the method will terminate in a finite number of steps, and is

guaranteed to give the correct answer. (If the condition number is poor enough, the "correct" answer is meaningless, due to roundoff error. A direct solve helps the conditioning problem, but doesn't get rid of it.) We developed a "fast" LU solve for a matrix which has been converted to a wavelet basis. It works the same way as a conventional LU solve, except we used the structure of the matrix to advantage to reduce the solve time to $\vartheta(N \ln N)$. The method is therefore as fast as iterative methods, and has the advantage of working better on ill-conditioned matrices. However, it must be emphasized that this does not solve the poor conditioning problem. Accuracy will still be lost due to round-off errors. Rather, it allows us to work with poorer conditioned matrices than we otherwise would. This work is summarized in the paper by Gines, et al. [3]

We also exploited the structure of the wavelet matrices in a second way. The matrices created by moment methods have a structure which depends on the numbering of the current discretization cells. This leads to banding of the matrices, in which there are bands and subbands of larger elements, and near zero entries between these bands. Conventional matrix solution techniques cannot take advantage of this structure. Indeed, the banding can actually be deleterious to the solve, in that a relatively sparse matrix can fill up in the process of getting the solution. We therefore developed a "two dimensional" wavelet method. The idea is that the wavelet method now knows about the banding. The matrix remains sparse during the solve; no fill in occurs. The method is summarized in Gines et al. [2]

1.2 Matrix Conditioning Methods

The matrices that are produced by commercial codes are typically very poorly conditioned. A poor condition number makes it difficult to quickly solve the matrix. The solve time of iterative methods goes as the condition number. In severe cases, it is not even possible to attain a solution when realistic computer roundoff error is considered. Poorly conditioned matrices will also hurt wavelet methods for matrix solutions. A wavelet transformation of the matrix is an orthogonal basis transformation, and the condition number will therefore be the same. This in turn means not many elements of the wavelet matrix may be thrown away, and sparsification of the matrix will not be that significant. Therefore, little speed up can be expected.

We examined the matrices and found the eigenvalue structure was not what we expected. Normally, a poorly conditioned matrix will have eigenvalues that decrease linearly with number, until the final eigenvalues are very small. The condition number is poor as it is the ratio of the largest to smallest eigenvalues. When we looked at the matrices from Momentum, we found that there two groups of eigenvalues. The first group had eigenvalues that were all about the same order of magnitude; the second group's eigenvalues were much smaller than the first group. This is an unusual eigenvalue structure and suggests that the underlying equations have a structure that can be exploited to improve the conditioning of the matrix. After some searching, we found that other researchers had similar ideas. In particular, we were influenced by the work of Vecchi et al [7]. In that work, Professor Vecchi explains how to precondition the matrices by breaking them up into two parts, and treating these two parts differently. The original matrix is converted to a new basis composed of "loops" and "stars". Loop basis functions represent a current which has no divergence; star basis functions have no curl. By breaking the current up in this manner, it is possible to correlate the loops and stars with the two groups of eigenvalues. This fact can be exploited to solve for the eigenvalues of the submatrices (loop - loop and star - star). The eigenvectors are used as a preconditioner, whereby the resulting matrix has a much better condition number.

Our contribution is to extend some of Vecchi's ideas to work more practically with the matrices we typically see in moment method codes. In particular, Vecchi's method relies on getting a static solution of the submatrices. We get the solution at the actual frequency of interest. We also believe we have a way of getting the eigenvalue structure without having to solve the complete submatrix problem. This work is still in progress, but promises to significantly increase the speed of the method. Details are given in the technical section of this report.

1.3 Fast Calculation of Parasitic Coupling in Packages

This work has been carried over from the other terminated MAFET contract. The purpose of the work is to be able to include parasitic coupling effects in circuit simulators. Parasitic coupling is defined to be unintended coupling between different parts of a circuit. It is difficult to include this kind of coupling in

a circuit simulator because it is usually not even known if the coupling exists or what it's level is. In earlier work, Dunn et. al [4] , developed coupling models between transmission lines in a circuit. The model consisted of an independent voltage and/or current source in the coupled line. That work had the limitation of needing a Green's function. Therefore, coupling inside a package cannot be calculated except for the academic exercise of an empty, rectangular box. This work extends the algorithm to include arbitrary package configurations. This is accomplished by not using a Green's function, but rather relying on field data from a finite element simulation code. In a sense, the finite element code generates a numerical Green's function.

We are still working on results for the method. Details are given in the technical section of the report.

2 Publications, Results, and Works in Progress

This section list the publications and talks resulting from this work. Work in progress is also discussed. No patents resulted in this contract.

2.1 Wavelet Methods

The principal document containing the wavelet work is David Gines Ph.D. thesis: [2] This work details the direct solve method, the two-dimensional wavelet method, and a host of examples.

The work on the direct solve method is also published in paper form as: [3]

The work on two-dimensional wavelets is being reworked in a more computationally desirable form. It is expected this work will be completed this academic year, at which point a paper will be published.

2.2 Matrix Conditioning Methods

This work is still in progress. The work completed to date has been presented in refereed conference publications: [6]

We will be presenting the latest results in a conference this spring [5]. We plan on submitting a full journal paper later this spring.

2.3 Fast Calculation of Parasitic Coupling in Packages

This work is still in progress. We plan on submitting a paper for publication later this spring.

3 Technical Description of Algorithms

We now present a technical description of the algorithms developed, especially for the work where publication is in progress.

3.1 Wavelet Methods

Since this work has been published [3, 2] , we only briefly describe it here. There are two main parts to this work: fast, direct solution of waveletized matrices; and a two dimensional wavelet algorithm.

The fast, direct solution method is now described. A full, dense matrix is converted to a wavelet basis in the standard manner. For details on this procedure, see for example [1]. In particular, we used the non-standard wavelet transformation, as described in that paper. The matrix produced has the standard wavelet structure, with groupings of submatrices following the diagonal. The matrices we obtained from Momentum are typically poorly conditioned; we therefore wanted a direct method. A normal LU decomposition on the matrix is not desirable as fill in will occur on the matrix, which is mainly zeros. The sparse, direct method developed overcomes this method by recognizing the block structure of the matrix and preserving it throughout the LU decomposition process. Pivoting is implemented within the blocks to keep the process conditionally convergent; thereby rendering it useful in poorly conditioned matrices examined in this work. Details are found in: [2]

The two dimensional wavelet algorithm again works on the waveletized version of the matrix. Each block of the matrix has subbanding associated with the numbering of the original cell basis of the problem. This numbering scheme is known, and therefore the subbanding is predictable. The two-dimensional scheme adds an extra set of indices to the wavelets. For example, we have four indices instead of the normal two for a one spatial dimensional problem; we have eight indices instead of four for a two spatial dimensional problem. This process is accomplished mathematically by working with matrices of matrices. The work was coded in C. The code is complicated because of the complicated indexing required. Benchmarks showed that the method will be faster for problem sizes above 5000 unknowns. Below that size, the method is actually slower, because of the increased overhead required in the indexing scheme. Details are given in: [2]

3.2 Matrix Conditioning Methods

The goal of this work is to be able to work with the poorly conditioned matrices resulting from the moment method solution. First, we understood the reason for the poor conditioning. We used the work of Vecchi [8], who understood the essential point. The integral equation used is an electric field integral equation (EFIE), in which there are two terms. We are solving for the unknown current on the signal lines. The first term, works on the divergence of the current, or equivalently the charge. The second term works on the whole current. The integral equation can have solutions which are nearly in the null space; i.e., near zero eigenvalues are possible. In particular, these eigenvalues result, because there are currents which have zero divergence. A zero divergence current is in the null space of the first term; the second term gives a contribution proportional to the frequency. Therefore, at low frequencies, the zero divergence current is nearly in the null space of the integral equation operators. This so called low frequency "catastrophe" is evident in all commercial planar solvers. Unfortunately, for most practical problems, we are close to this limit. Even if a solution is possible, it is impossible to use iterative solvers, and sparsification techniques, for example wavelet methods, will do little good.

Fortunately, in Vechhi's paper a method is suggested to fix the problem. Specifically, a preconditioner is developed whereby the condition number of the transformed matrix is lowered substantially. The gist of the method is to rewrite the current into two different sets of basis functions: divergence free and curl free. These functions are usually referred to as loops (divergence free) and stars (curl free). This transformation on the matrix is useful to carry out because of the two terms in the integral equation. The first term only operates on the loops; the second term operates on both the loops and the stars. Vecchi showed that the resulting matrix has a very clear structure, in which the star-star part is dominant, and the loop-loop part is nearly (but not totally) independent. This suggests a preconditioner. An electrostatic solve of the problem is made. This works only on the charge, or star-star part of the matrix. This problem can be solved using fast, electrostatic methods. The resulting eigenfunctions can be used as a new basis for the star part of the current. Only a few are needed. The loop-loop part of the problem is preconditioned in the same way. A magnetostatic solve is carried out, with the resulting eigenfunctions being used as the preconditioning basis. Vecchi has demonstrated that the method works well for patch antenna problems.

Vecchi's method has some drawbacks for our applications. First of all, he requires a static solve of the problem, which is awkward when we are trying to use solutions from commercial codes. Second, the static solves can take $\vartheta(N^3)$ amount of time. The method is therefore expensive to run. It does bring down the condition number, but only results in time savings if several frequency points are used, and the same basis can be reused. We therefore set out to solve these two drawbacks. The first problem is overcome by taking the star-star and loop-loop blocks of the matrix and performing a singular value decomposition on them (SVD). This method allows us to get preconditioning bases at the frequencies of interest without having to use a static solution. We then reuse the basis over the frequency band of interest. Benchmarks show that the method is useful in reducing the condition number over the frequency band of interest, with one caveat. It is difficult to go through a resonance in the frequency response of the circuit. Details are given in: [5]. This solution fixes with static solve issue, but we still have speed problems. SVD is a very expensive algorithm: $\vartheta(5N^3)$. Fortunately, we only have to run it at one frequency in our band. We have a new idea how to better solve this problem. We are investigating using QR algorithm, instead of SVD. The advantage of this is that the QR algorithm gives us the most "important" eigenvalues and eigenvectors first. We don't need to get all the eigenvalues. Recall that the final basis has only a few dominant terms. We can get these terms first,

and stop the algorithm quickly. This is the same idea as is used in some image compression techniques. The question is whether QR is stable for the matrices we are using. We think it will be, but we still have to test the procedure. We hope to have definitive results by later this spring.

3.3 Fast Calculation of Parasitic Coupling in Packages

The algorithm is based on previous work by Dunn [4]. A method is described in that paper where the coupling between two arbitrary oriented lines on a substrate is calculated. The algorithm works by exciting one of the lines, and observing the fields it produces at the other line. These fields produce voltages and currents in the second line. These same voltages and currents can be reproduced by modeling the coupling as independent voltage and current sources in the second line. The model is approximate in that no interaction back to the first line is accounted for, and energy is not conserved in the sense that the independent voltage and current sources create energy. Nonetheless, it can be a useful approximation if the coupling is relatively weak, is as typically the case in parasitic coupling problems. The independent voltage and current sources can be placed in a circuit simulation package, and give the designer an idea if coupling is a problem.

The main drawback of this work is that it requires a Green's function in order to calculate the fields at the second line. Therefore, generalized packages are not allowed. We have generalized the method by using a finite element program (HP-HFSS) to calculate the fields from the first line. The fields can be extracted anywhere in the space of the simulation, in particular where the second line is. The independent voltage and current sources are then calculated. An integration is carried out over the second line, where the magnetic or electric field from the first line is in the integrand. The method is limited in the accuracy obtained for the fields. Typically, large tetrahedra are used in a region where the second line exists. We are still testing the method on a variety of canonical structures. Preliminary data show that the method works well enough that order of magnitude estimates of coupling problems can be made. Notice, that the advantage of this method over having the finite element program simply calculate the coupling between two lines, is that now the second line can be anywhere in the package. Only one simulation need be carried out per package. This is in contrast to requiring a new simulation every time the second line is moved. We expect to be publishing the results later this spring.

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